

Citation for published version:

Papadopoulos, TA, Muccioli, L, Athanasopoulos, S, Walker, AB, Zannoni, C & Beljonne, D 2011, 'Does supramolecular ordering influence exciton transport in conjugated systems? Insight from atomistic simulations', *Chemical Science*, vol. 2, no. 6, pp. 1025-1032. <https://doi.org/10.1039/c0sc00467g>

DOI:

[10.1039/c0sc00467g](https://doi.org/10.1039/c0sc00467g)

Publication date:

2011

[Link to publication](https://doi.org/10.1039/c0sc00467g)

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1 † Electronic Supplementary Information (ESI)

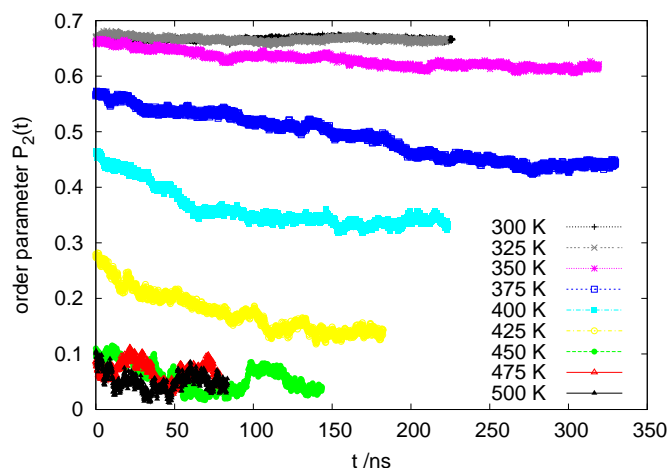


Fig. ESI 1 Evolution of the nematic order parameter during the equilibration phase of the 256-molecule samples.

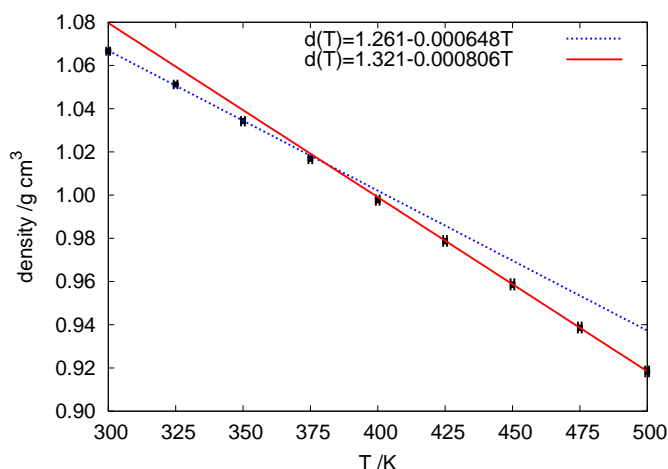


Fig. ESI 2 Simulated temperature behaviour of the density in the smectic (low T) and isotropic (high T) phase. In each phase, the temperature dependence follows a linear trend; the least square fitting lines and parameters are also reported. The two lines intersect at $T=379.7$ K

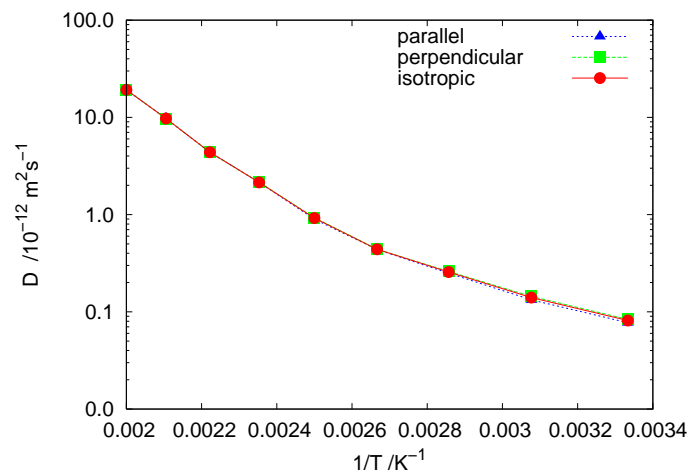


Fig. ESI 3 Arrhenius plot of the translational diffusion coefficient, calculated from the mean square displacements of the centers of mass ($D_{ii} = \langle [r_i(t) - r_i(0)]^2 \rangle / 2t$, $t=10$ ns, $i=x,y,z$, $D_{\perp} = (D_{xx} + D_{yy})/2$, $D_{\parallel} = D_{zz}$). The diffusion is fairly isotropic also in the smectic phase, but the phase change is revealed by the two separate regions with different activation energy.

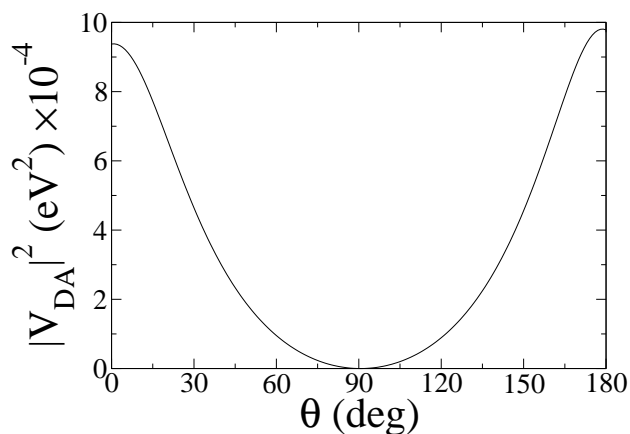


Fig. ESI 4 The squared excitonic coupling $|V_{DA}|^2$ between two chromophores as a function of their relative orientation and distance of 8.5\AA , which corresponds to the average distance between first nearest neighbors within the smectic layers at 300 K.

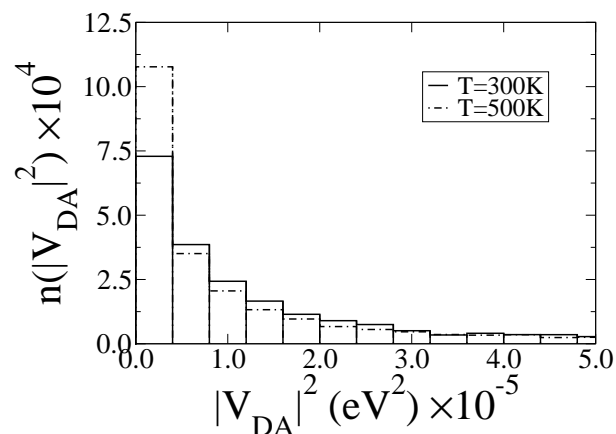


Fig. ESI 5 The distribution of the squared excitonic coupling $|V_{DA}|^2$ for $T=300\text{K}$ and $T=500\text{K}$.

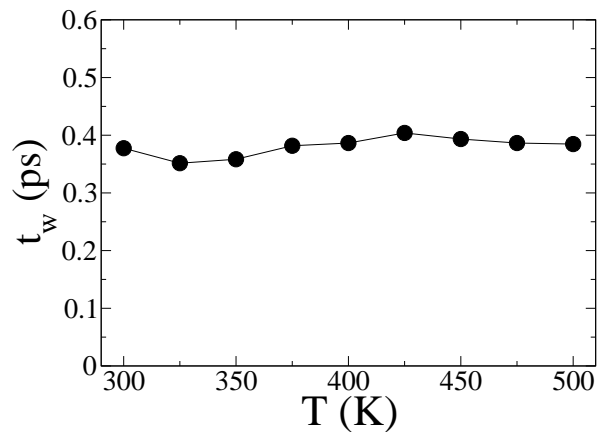


Fig. ESI 6 The average waiting time of the exciton as a function of temperature.

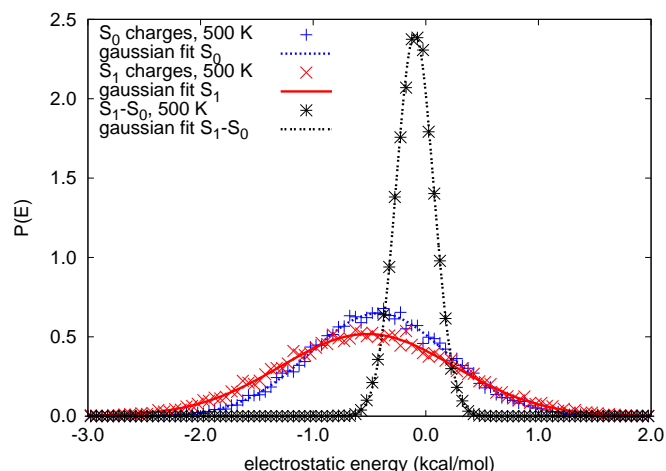


Fig. ESI 7 The electrostatic disorder distribution at 500 K. The distributions for the ground and excited states correspond to calculation of the electrostatic interaction between a molecule and all its neighbours using the ground state and excited state atomic charges, respectively. The difference distribution is instead the difference between ground and excited state electrostatic energy calculated for the same molecule. The standard deviations are $\sigma_0 = 0.62$ kcal/mol (0.0267 eV), $\sigma_1 = 0.77$ kcal/mol (0.0334 eV), $\sigma_{1-0} = 0.166$ kcal/mol (0.007 eV). The difference distribution between two arbitrary molecules instead should have standard deviation $\sigma_{1,i-0,j} = (\sigma_1^2 + \sigma_0^2)^{1/2} = 0.99$ kcal/mol (0.0429 eV). All deviations are of the order or even smaller than the thermal energy at 500 K which corresponds to 0.994 kcal/mol (0.04308 eV).

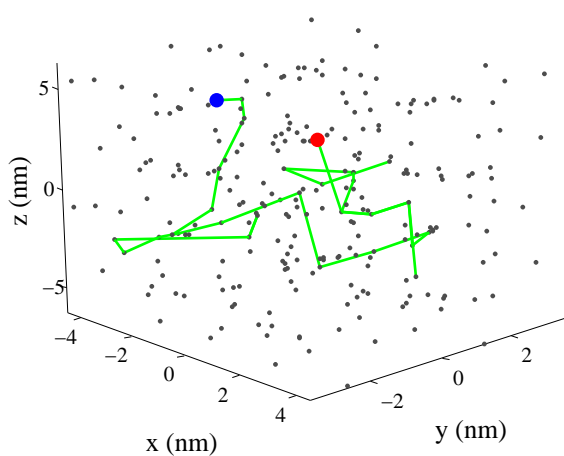


Fig. ESI 8 A trajectory of an exciton as it hops from the site of creation (blue) until the site where it recombines (red).